1,3,5-Cycloheptatriene

Other names:	Cyclohepta-1,3,5-triene
	Cycloheptatriene
	Tropilidene
	Tropilidin
	UN 2603
Inchi:	InChI=1S/C7H8/c1-2-4-6-7-5-3-1/h1-6H,7H2
InchiKey:	CHVJITGCYZJHLR-UHFFFAOYSA-N
Formula:	C7H8
SMILES:	C1=CC=CCC=C1
Mol. weight [g/mol]:	92.14
CAS:	544-25-2

Physical Properties

Property code	Value	Unit	Source
chl	-4040.00 ± 2.00	kJ/mol	NIST Webbook
gf	118.00	kJ/mol	Joback Method
hf	187.00	kJ/mol	NIST Webbook
hfus	6.22	kJ/mol	Joback Method
hvap	38.70 ± 0.21	kJ/mol	NIST Webbook
hvap	38.70 ± 0.20	kJ/mol	NIST Webbook
ie	8.28	eV	NIST Webbook
ie	8.03	eV	NIST Webbook
ie	8.20 ± 0.05	eV	NIST Webbook
ie	8.50	eV	NIST Webbook
ie	8.52	eV	NIST Webbook
ie	8.40	eV	NIST Webbook
ie	8.29	eV	NIST Webbook
log10ws	-2.15		Aqueous Solubility Prediction Method
logp	2.059		Crippen Method
mcvol	85.730	ml/mol	McGowan Method
pc	4333.96	kPa	Joback Method
rinpol	784.00		NIST Webbook
rinpol	787.00		NIST Webbook
rinpol	758.00		NIST Webbook
rinpol	765.00		NIST Webbook
rinpol	776.00		NIST Webbook

rinpol	784.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	772.00		NIST Webbook
rinpol	108.90		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	785.00		NIST Webbook
rinpol	775.00		NIST Webbook
rinpol	769.00		NIST Webbook
rinpol	763.00		NIST Webbook
rinpol	756.00		NIST Webbook
rinpol	774.00		NIST Webbook
rinpol	786.60		NIST Webbook
rinpol	782.60		NIST Webbook
rinpol	784.00		NIST Webbook
rinpol	794.00		NIST Webbook
rinpol	807.00		NIST Webbook
rinpol	800.00		NIST Webbook
rinpol	108.90		NIST Webbook
rinpol	771.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1056.00		NIST Webbook
ripol	1089.00		NIST Webbook
ripol	1089.00		NIST Webbook
sg	315.60 ± 1.10	J/mol×K	NIST Webbook
sl	214.64	J/mol×K	NIST Webbook
tb	389.70	K	NIST Webbook
tc	604.64	K	Joback Method
tf	193.40	K	Aqueous Solubility Prediction Method
tt	197.91 ± 0.07	K	NIST Webbook
tt	197.92 ± 0.05	K	NIST Webbook
tt	197.92 ± 0.07	K	NIST Webbook
vc	0.311	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	201.05	J/mol×K	604.64	Joback Method
cpg	191.71	J/mol×K	568.12	Joback Method
cpg	181.69	J/mol×K	531.60	Joback Method
cpg	170.98	J/mol×K	495.08	Joback Method
cpg	159.55	J/mol×K	458.57	Joback Method
cpg	147.36	J/mol×K	422.05	Joback Method
cpg	134.40	J/mol×K	385.53	Joback Method
cpl	162.76	J/mol×K	298.15	NIST Webbook
dvisc	0.0099693	Pa×s	179.03	Joback Method
dvisc	0.0013955	Pa×s	247.86	Joback Method
dvisc	0.0007480	Pa×s	282.28	Joback Method
dvisc	0.0031831	Pa×s	213.45	Joback Method
dvisc	0.0003102	Pa×s	351.11	Joback Method
dvisc	0.0002247	Pa×s	385.53	Joback Method
dvisc	0.0004592	Pa×s	316.70	Joback Method
hfust	1.16	kJ/mol	198.00	NIST Webbook
hfust	1.16	kJ/mol	198.00	NIST Webbook
hfust	2.35	kJ/mol	154.00	NIST Webbook
hvapt	39.40	kJ/mol	344.50	NIST Webbook
hvapt	40.80	kJ/mol	305.50	NIST Webbook
sfust	15.24	J/mol×K	154.00	NIST Webbook
sfust	5.86	J/mol×K	198.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	390.20	K	99.90	NIST Webbook
tbrp	333.70	K	16.30	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.50540e+01
Coeff. B	-3.87828e+03
Coeff. C	-1.80620e+01
Temperature range (K), min.	280.70

Temperature range (K), max.	416.14

Sources

Relation between characteristic molecular volume and hydrophobicity of nonpolar molecules:	https://www.doi.org/10.1016/j.jct.2010.04.011
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C544252&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
sl:	Liquid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature

tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume